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STRUCTURE FILE UPDATES: 22 NOV 2004 HIGHEST RN 786612-66-6
 DICTIONARY FILE UPDATES: 22 NOV 2004 HIGHEST RN 786612-66-6

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

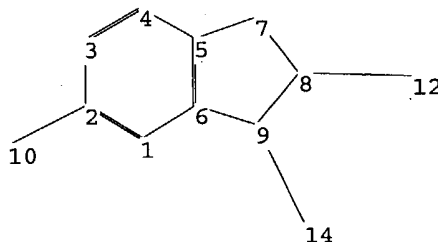
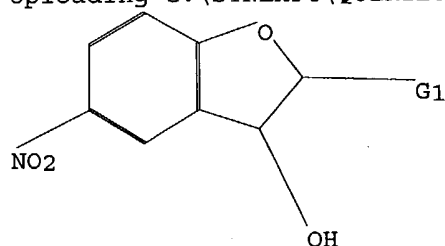
Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=>

Uploading C:\STNEXP4\QUERIES\10-642947z.str



chain nodes :
 10 12 14
 ring nodes :
 1 2 3 4 5 6 7 8 9
 chain bonds :
 2-10 8-12 9-14
 ring bonds :
 1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9
 exact/norm bonds :
 8-12 9-14
 exact bonds :
 2-10 5-7 6-9 7-8 8-9
 normalized bonds :
 1-2 1-6 2-3 3-4 4-5 5-6
 isolated ring systems :
 containing 1 :

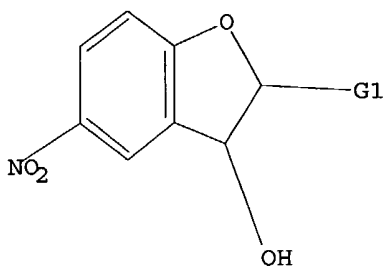
G1:H,C

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS
 12:CLASS 14:CLASS

L1 STRUCTURE UPLOADED

=> d
 L1 HAS NO ANSWERS
 L1 STR



G1 H,C

Structure attributes must be viewed using STN Express query preparation.

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 FULL SEARCH INITIATED 13:37:22 FILE 'REGISTRY'
 FULL SCREEN SEARCH COMPLETED - 855 TO ITERATE

100.0% PROCESSED 855 ITERATIONS 20 ANSWERS
 SEARCH TIME: 00.00.01

L2 20 SEA SSS FUL L1

=> fil caplus		
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	155.42	155.63

FILE 'CAPLUS' ENTERED AT 13:37:27 ON 23 NOV 2004
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FILE COVERS 1907 - 23 Nov 2004 VOL 141 ISS 22
 FILE LAST UPDATED: 22 Nov 2004 (20041122/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

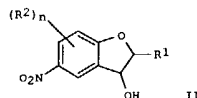
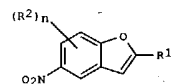
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 L3 7 L2

L3 ANSWER 1 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 2004:142849 CAPLUS
 DOCUMENT NUMBER: 140:181316
 TITLE:

INVENTOR(S):
 PATENT ASSIGNEE(S):
 SOURCE:
 DOCUMENT TYPE:
 LANGUAGE:
 FAMILY ACC. NUM. COUNT:
 PATENT INFORMATION:

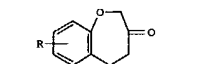
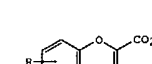
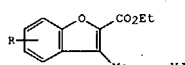
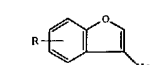
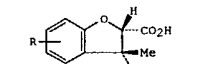
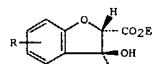
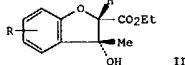
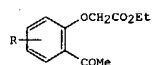
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US 2004034220	A1	20040219	US 2003-642947	20030818
DE 10237819	A1	20040304	DE 2002-10237819	20020819
EP 1394155	A2	20040303	EP 2003-17811	20030805
EP 1394155	A3	20040324		
R: AF, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
CN 1485323	A	20040331	CN 2003-154803	20030819
PRIORITY APPLN. INFO.: DE 2002-10237819 A 20020819				

OTHER SOURCE(S): MARPAT 140:181316
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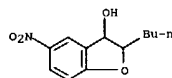
AB The invention relates to a process for preparation 5-nitrobenzofurans I by dehydration of 5-nitro-2,3-dihydrobenzofuran-3-ols II in the presence of protic acids or hydroxides [wherein R1 = H, alkyl; R2 = independently F, Cl, Br, I, alkyl, OH and derivs., NH2 and derivs., CONH2 and derivs.; n = 0-3; or when n = 2, 3 it is possible that R2CCR2 = (un)substituted ring; with the proviso of 2-(n-butyl)-5-nitrobenzofuran be excluded] were prepared as new active compds. for treating cardiac arrhythmias. The advantages include low-cost, stable and easily obtainable precursors, higher product yields, and minimization of waste. For example, 2-(n-butyl)-5-nitrobenzofuran was prepared, in 80% yield, by dehydration of 2-(n-butyl)-5-nitro-2,3-dihydrobenzofuran-3-ol (III) in EtOH in the presence of concentrated H2SO4 at reflux for 4 h. III was prepared in 6 steps by O-alkylation of Me salicylate with methyl-2-bromohexanoate,

L3 ANSWER 2 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 1992:448242 CAPLUS
 DOCUMENT NUMBER: 117:48242
 TITLE: Benzofuran derivatives. Part 4. Synthesis of benzofurans and 2,3,4,5-tetrahydro-1-benzoxepin-3,5-diones
 AUTHOR(S): Suzuki, Tsuneo; Tanemura, Kiyoshi; Horaguchi, Takaaki;
 CORPORATE SOURCE: Shimizu, Takahachi; Sakakibara, Toku
 Sch. Den. Niigata, Nippon Dent. Univ., Hamaura, 951, Japan
 SOURCE: Journal of Heterocyclic Chemistry (1992), 29(2), 423-9
 CODEN: JHCTAD; ISSN: 0022-152X
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



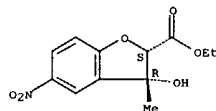
AB By treatment of Et 4- or 5-substituted 2-acetylphenoxycetates I (R = 4-Me, H, 5-Cl, etc.) with potassium hydroxide in dry dioxane, benzofurans II-VII and 2,3,4,5-tetrahydro-1-benzoxepin-3,5-diones VIII were obtained. The relative yields of benzofurans II-VII and 2,3,4,5-tetrahydro-1-benzoxepin-3,5-diones VIII varied with the types of 4- or 5-substituents. The electron-donating 4-methoxy group favored the formation of benzofurans. On the other hand, electron-withdrawing substituents such as the 4-nitro group favored the formation of benzofurans. When esters I were treated with sodium amide, 2,3-dihydrobenzofurans II were obtained exclusively regardless of 4- or 5-substituents.

L3 ANSWER 1 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
 NaOH-hydrolysis, cyclizing decarboxylation of 2-(1-carboxypentoxyl)benzoic acid, HCl-hydrolysis, nitration in the presence of HNO3/H2SO4, and redn. with NaBH4 in ethanol.
 IT 658053-39-5P, 2-(n-Butyl)-5-nitro-2,3-dihydrobenzofuran-3-ol
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 dehydration of 5-nitro-2,3-dihydrobenzofuran-3-ols in the presence of protic acids or hydroxides
 RN 658053-39-5 CAPLUS
 CN 3-Benzofuranol, 2-butyl-2,3-dihydro-5-nitro- (9CI) (CA INDEX NAME)



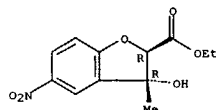
L3 ANSWER 2 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
 IT 104862-17-1P 104862-21-7P 104862-25-1P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 RN 104862-17-1 CAPLUS
 CN 2-Benzofuran-3-carboxylic acid, 2,3-dihydro-3-hydroxy-3-methyl-5-nitro-, ethyl ester, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



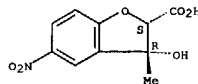
RN 104862-21-7 CAPLUS
 CN 2-Benzofuran-3-carboxylic acid, 2,3-dihydro-3-hydroxy-3-methyl-5-nitro-, ethyl ester, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



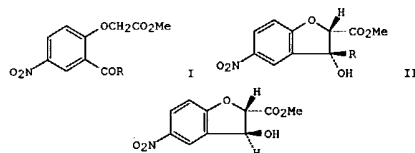
RN 104862-25-1 CAPLUS
 CN 2-Benzofuran-3-carboxylic acid, 2,3-dihydro-3-hydroxy-3-methyl-5-nitro-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L3 ANSWER 3 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 1989:94892 CAPLUS
 DOCUMENT NUMBER: 110:94892
 TITLE: The cyclization reaction of methyl
 2-acyl-4-nitrophenoxycetates with potassium

hydroxide
 AUTHOR(S): Suzuki, Tsuneo
 Sch. Dent., Nippon Dent. Univ., Niigata, 951, Japan
 CORPORATE SOURCE: Nippon Shika Daigaku Kiyo, Ippan Kyoiku-kei (1988),
 17, 111-18
 CODEN: NSDKDD; ISSN: 0385-1605
 JOURNAL
 LANGUAGE: English
 GI



III

AB Cyclization of nitrophenoxycetate I (R = H) with KOH in dioxane gave a mixture of cis- and trans-benzofurancarboxylates II (R = H) and III, resp.

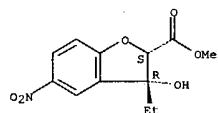
Similar cyclization of I (R = Me, Et, CHMe2) gave only 'cis products II (R = Me, Et, CHMe2).

IT 104862-29-5 104862-30-8 119197-60-1
 119197-69-2 119197-70-5 119197-71-6
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (cyclization of, with potassium hydroxide, stereochem. of)

RN 104862-29-5 CAPLUS
 CN 2-Benzofurancarboxylic acid, 2,3-dihydro-3-hydroxy-3-methyl-5-nitro-, methyl ester, cis- (9CI) (CA INDEX NAME)

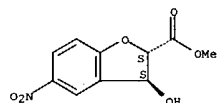
Relative stereochemistry.

L3 ANSWER 3 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



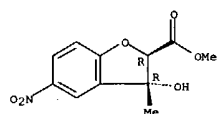
RN 119197-70-5 CAPLUS
 CN 2-Benzofurancarboxylic acid, 2,3-dihydro-3-hydroxy-5-nitro-, methyl ester, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 119197-71-6 CAPLUS
 CN 2-Benzofurancarboxylic acid, 2,3-dihydro-3-hydroxy-3-methyl-5-nitro-, methyl ester, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.

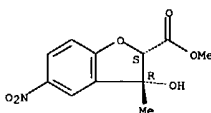


IT 104862-25-1P 104862-26-2P 119197-72-7P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and esterification of, with diazomethane)

RN 104862-25-1 CAPLUS
 CN 2-Benzofurancarboxylic acid, 2,3-dihydro-3-hydroxy-3-methyl-5-nitro-, cis- (9CI) (CA INDEX NAME)

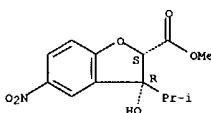
Relative stereochemistry.

L3 ANSWER 3 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



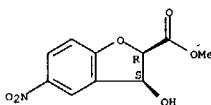
RN 104862-30-8 CAPLUS
 CN 2-Benzofurancarboxylic acid, 2,3-dihydro-3-hydroxy-3-(1-methylethyl)-5-nitro-, methyl ester, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 119197-68-1 CAPLUS
 CN 2-Benzofurancarboxylic acid, 2,3-dihydro-3-hydroxy-5-nitro-, methyl ester, cis- (9CI) (CA INDEX NAME)

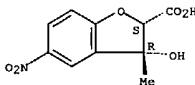
Relative stereochemistry.



RN 119197-69-2 CAPLUS
 CN 2-Benzofurancarboxylic acid, 3-ethyl-2,3-dihydro-3-hydroxy-5-nitro-, methyl ester, cis- (9CI) (CA INDEX NAME)

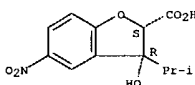
Relative stereochemistry.

L3 ANSWER 3 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



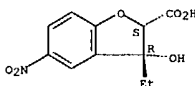
RN 104862-26-2 CAPLUS
 CN 2-Benzofurancarboxylic acid, 2,3-dihydro-3-hydroxy-3-(1-methylethyl)-5-nitro-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.

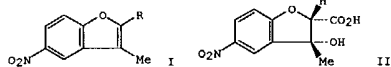


RN 119197-72-7 CAPLUS
 CN 2-Benzofurancarboxylic acid, 3-ethyl-2,3-dihydro-3-hydroxy-5-nitro-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L3 ANSWER 4 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 1988:75142 CAPLUS
 DOCUMENT NUMBER: 108:75142
 TITLE: Benzofuran derivatives. Part 3. The reactivities of the intermediates in benzofuran synthesis
 AUTHOR(S): Horaguchi, Takaaki; Matsuda, Shinichi; Tanemura, Kiyoshi; Suzuki, Tsuneo
 CORPORATE SOURCE: Fac. Sci., Niigata Univ., Niigata, 950-21, Japan
 SOURCE: Journal of Heterocyclic Chemistry (1987), 24(4), 965-9
 CODEN: JHTCAD; ISSN: 0022-152X
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 108:75142
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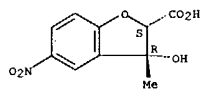
AB 3-Methyl-5-nitrobenzofuran (I, R = H) and 3-methyl-5-nitrobenzofuran-2-carboxylic acid (I, R = CO₂H) were obtained by heating 2,4-Ac(NO₂)C₆H₃OCH₂CO₂H with various bases in Ac₂O. It appeared that 3-hydroxy-3-methyl-5-nitro-2,3-dihydrobenzofuran-2-carboxylic acid (II) was the intermediate in the benzofuran synthesis. The properties of II were examined under various conditions. Using strong bases such as Et₃N

in place of NaOAc, I (R = CO₂H) was obtained exclusively. However, in the presence of NaOAc, I (R = H) was obtained in good yield. The reaction pathways for the formation of I (R = H, CO₂H) are discussed.

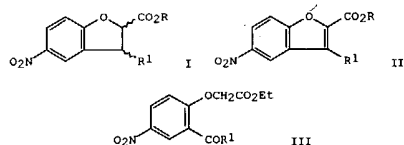
IT 104862-25-1P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation, decarboxylation, and dehydration of)

RN 104862-25-1 CAPLUS
 CN 2-Benzofurancarboxylic acid, 2,3-dihydro-3-hydroxy-3-methyl-5-nitro-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L3 ANSWER 5 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 1986:590808 CAPLUS
 DOCUMENT NUMBER: 105:190808
 TITLE: Benzofuran derivatives. II. Synthesis of 2,3-dihydrobenzofurans from ethyl 2-acylphenoxyacetates
 AUTHOR(S): Suzuki, Tsuneo
 CORPORATE SOURCE: Nippon Dent. Univ. Niigata, Niigata, 951, Japan
 SOURCE: Bulletin of the Chemical Society of Japan (1985), 58(10), 2821-5
 CODEN: BCSJAB; ISSN: 0009-2673
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 105:190808
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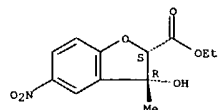
AB Benzofurancarboxylates I and II (R = H, Et; R₁ = H, Me, Et, CHMe₂) were obtained from the reaction of Et (2-acyl-4-nitrophenoxy)acetates III with KOH in dry dioxane. The relative ratios of the cis and trans isomers

with respect to C-2 and C-3 stereochem. varied according to the structure of the acyl group. When the acyl group was acetyl, propionyl, or isobutyryl group, the cis isomers were exclusively obtained in high yields. On the other hand, a near equimol. amount of the cis and trans isomers was obtained from the reaction of 2-formyl derivs. under the same conditions.

IT 104862-17-1P 104862-21-7P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and reaction of, with potassium hydroxide)

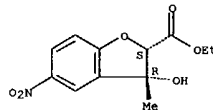
RN 104862-17-1 CAPLUS
 CN 2-Benzofurancarboxylic acid, 2,3-dihydro-3-hydroxy-3-methyl-5-nitro-, ethyl ester, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



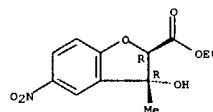
L3 ANSWER 4 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
 IT 104862-17-1P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation, saponification, acylation, and dehydration of)
 RN 104862-17-1 CAPLUS
 CN 2-Benzofurancarboxylic acid, 2,3-dihydro-3-hydroxy-3-methyl-5-nitro-, ethyl ester, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L3 ANSWER 5 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
 RN 104862-21-7 CAPLUS
 CN 2-Benzofurancarboxylic acid, 2,3-dihydro-3-hydroxy-3-methyl-5-nitro-, ethyl ester, trans- (9CI) (CA INDEX NAME)

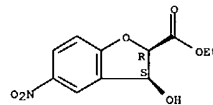
Relative stereochemistry.



IT 104862-16-0P 104862-18-2P 104862-19-3P
 104862-20-6P 104862-25-1P 104862-26-2P
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 (preparation of)

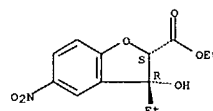
RN 104862-16-0 CAPLUS
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Relative stereochemistry.



RN 104862-18-2 CAPLUS
 CN 2-Benzofurancarboxylic acid, 3-ethyl-2,3-dihydro-3-hydroxy-5-nitro-, ethyl ester, cis- (9CI) (CA INDEX NAME)

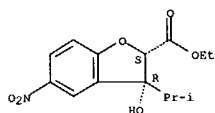
Relative stereochemistry.



RN 104862-19-3 CAPLUS
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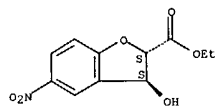
Relative stereochemistry.

L3 ANSWER 5 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



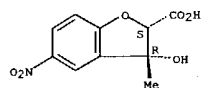
RN 104862-20-6 CAPLUS
 CN 2-Benzofurancarboxylic acid, 2,3-dihydro-3-hydroxy-5-nitro-, ethyl ester, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



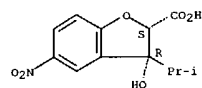
RN 104862-25-1 CAPLUS
 CN 2-Benzofurancarboxylic acid, 2,3-dihydro-3-hydroxy-3-methyl-5-nitro-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 104862-26-2 CAPLUS
 CN 2-Benzofurancarboxylic acid, 2,3-dihydro-3-hydroxy-3-(1-methylethyl)-5-nitro-, cis- (9CI) (CA INDEX NAME)

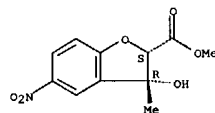
Relative stereochemistry.



RN 104862-29-5 CAPLUS

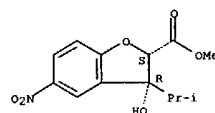
L3 ANSWER 5 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
 CN 2-Benzofurancarboxylic acid, 2,3-dihydro-3-hydroxy-3-methyl-5-nitro-, methyl ester, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 104862-30-8 CAPLUS
 CN 2-Benzofurancarboxylic acid, 2,3-dihydro-3-hydroxy-3-(1-methylethyl)-5-nitro-, methyl ester, cis- (9CI) (CA INDEX NAME)

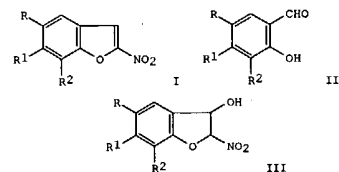
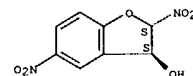
Relative stereochemistry.



L3 ANSWER 6 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1986:552861 CAPLUS
 DOCUMENT NUMBER: 105:152861
 TITLE: An improved synthesis of 2-nitrobenzo[b]furans
 AUTHOR(S): Tromelin, Anne; Demerseman, Pierre; Royer, Rene
 CORPORATE SOURCE: Serv. Chim., Inst. Curie, Paris, F-75231, Fr.
 SOURCE: Synthesis (1985), (11), 1074-6
 CODEN: SYNIBF; ISSN: 0039-7881
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 105:152861
 GI

L3 ANSWER 6 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

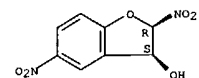


AB Ten nitrobenzofurans I (R = H, MeO, Br, NO₂, MeCO, CO₂Me, cyano; R₁ = H, MeO; R₂ = H, MeO, Br) were prepared in 2 steps by treating hydroxybenzaldehydes II with BrCH₂NO₂ and K₂CO₃ in Me₂CO to give 48-97% hydroxynitrodihydrobenzofurans III which were dehydrated in refluxing

Ac₂O to quant. give I.
 IT 104412-87-5P 104412-95-5P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and dehydration of)

RN 104412-87-5 CAPLUS
 CN 3-Benzofuranol, 2,3-dihydro-2,5-dinitro-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 104412-95-5 CAPLUS
 CN 3-Benzofuranol, 2,3-dihydro-2,5-dinitro-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.

L3 ANSWER 7 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1967:411444 CAPLUS
DOCUMENT NUMBER: 67:11444
TITLE: Benzo-furanooxazines
AUTHOR(S): Hill, John; Ramage, George R.
CORPORATE SOURCE: Univ. Salford, Salford, UK
SOURCE: Journal of the Chemical Society [Section] C: Organic
(1967), (8), 783-4
CODEN: JSCOAX; ISSN: 0022-4952
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 67:11444
GI For diagram(s), see printed CA issue.
AB Syntheses of 7-acetyl-3,4-dihydro-3,6-dimethyl-2H-benzofurano-[6,5-b][1,4]oxazine (I) and related compds. are described.
IT 14742-06-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 14742-06-4 CAPLUS
CN 2-Propanone, 1-[(2-acetyl-2,3-dihydro-3-hydroxy-3-methyl-5-nitro-6-benzofuranyl)oxy]- (8CI) (CA INDEX NAME)

